

WHAT IS CLAIMED IS:

1. An automated apparatus for performing reaction kinetics studies, the apparatus comprising:

a plurality of reaction blocks including at least one hot reaction block for heating one or more reaction vessels and at least one cold reaction block for cooling the one or more reaction vessels after heating thereof;

a robotic device for transferring one reaction vessel from one hot reaction block to one cold reaction block; and

a controller having a user interface for inputting a predetermined temperature profile and a predetermined sampling interval, the controller being in communication with the plurality of reaction blocks and the robotic device so as to instruct the robotic device to transfer one reaction vessel from one hot reaction block to one cold reaction block at a predefined transfer time within the predetermined sampling interval, the predetermined temperature profile representing the temperature of at least one of the hot reaction blocks over a time period of the study.

2. The apparatus of claim 1, wherein each of the hot and cold reaction blocks has a plurality of openings formed therein, one opening receiving one reaction vessel.

1 3. The apparatus of claim 1, further including:
2 a heating device associated with each of the hot reaction blocks for controlled heating
3 thereof; and
4 a cooling device associated with each of the cold reaction blocks for controlled
5 cooling thereof, wherein each of the heating and cooling devices is in communication with the
6 controller.

1 4. The apparatus of claim 3, wherein the heating device heats the hot
2 reaction blocks according to the predetermined temperature profile.

1 5. The apparatus of claim 1, wherein the predetermined temperature
2 profile includes an initial temperature and a final temperature, the predetermined temperature profile
3 being defined by the initial temperature and the final temperature.

1 6. The apparatus of claim 1, wherein the predetermined sampling interval
2 includes a study start time and a study stop time with the sampling interval being the time period
3 beginning with the start time and ending with the stop time of the study.

1 7. The apparatus of claim 1, wherein the robotic device moves in three
2 dimensions relative to the plurality of reaction blocks so as to permit the robotic device to grasp and
3 transfer the plurality of reaction vessels.

1 8. The apparatus of claim 1, wherein the robotic device has a gripping
2 mechanism for gripping and transferring one reaction vessel from the hot reaction block to the cold
3 reaction block at the predefined transfer time.

1 9. The apparatus of claim 8, wherein the gripping mechanism is operated
2 by toggling a predetermined pressure between first and second lines such that the gripping
3 mechanism closes to securely engage one reaction vessel for transfer from the hot reaction block to
4 the cold reaction block when a pressure is applied to the first line with the second line being vented,
5 the gripping mechanism opening to release the one reaction vessel when the pressure is applied to
6 the second line with the first line being vented.

1 10. The apparatus of claim 8, wherein the gripping mechanism includes a
2 first finger and a second opposing finger with a space therebetween, one reaction vessel being
3 disposed within the space and held between the first and second fingers during the transfer of the one
4 reaction vessel from the hot reaction block to the cold reaction block.

1 11. The apparatus of claim 1, wherein the controller includes a master
2 clock and a count-down clock, the master clock displaying the sampling interval for the study and
3 the count-down clock counting down the time before the next transfer of one of the reaction vessels.

1 12. The apparatus of claim 1, wherein the master controller includes a user
2 interface for inputting the predetermined temperature profile and the predetermined sampling
3 interval.

1 13. The apparatus of claim 1, further including:
2 a temperature control device operatively connected to one or more of the hot
3 and cold reaction blocks for controlling a temperature of each of the hot and cold reaction blocks,
4 the temperature control device being in communication with the controller, and
5 a temperature monitoring device for monitoring the temperature within at least
6 one of the hot and cold blocks, the temperature monitoring device being in communication with the
7 controller so as to provide the controller with temperature data representing the temperature of one
8 or more of the hot and cold blocks.

1 14. The apparatus of claim 11, wherein ^{112nd} the temperature control device
2 comprises one of a single loop, dual loop, and multi-loop temperature controller.

1 15. The apparatus of claim 11, wherein ^{112nd} the temperature monitoring device /
2 is a resistance temperature detector.

1 16. The apparatus of claim 1, wherein the predetermined temperature
2 profile is an isothermal temperature profile

1 17. The apparatus of claim 1, wherein the predetermined temperature
2 profile is a nonisothermal temperature profile.

1 18. An automated apparatus for performing reaction kinetics studies, the
2 apparatus comprising:
3 a plurality of reaction blocks including at least one hot reaction block for heating one
4 or more reaction vessels and at least one cold reaction block for cooling the one or more reaction
5 vessels after heating thereof;
6 a robotic device for transferring one reaction vessel from one hot reaction block to
7 one cold reaction block;

a controller having a user interface for inputting at least (1) a number of reaction vessels for the study, (2) a first predetermined temperature profile and (3) a predetermined study time period beginning with a start time and ending with a stop time, wherein the controller is in communication with the hot and cold reaction blocks and the robotic device, the controller including an operating system which instructs the robotic device to transfer the plurality of reaction vessels from one hot reaction block to one cold reaction block at predefined transfer times and wherein at least one of the hot reaction blocks is heated according to the first predetermined temperature profile over the study time period, the controller collecting and storing kinetics data for each reaction vessel transfer, the kinetics data at least (including) a temperature of the hot reaction block at each transfer time (and) a sampling time when each reaction vessel transfer from the hot reaction block to the cold reaction block occurred.

19. The apparatus of claim 18, wherein the hot reaction block has a number of openings formed therein for receiving a number of reaction vessels, the hot reaction blocks being connected to one or more heating devices with one or more temperature control devices being associated with the one or more heating devices for setting the temperature of one or more hot reaction blocks and wherein each cold reaction block has a number of openings formed therein for receiving a number of reaction vessels, the cold reaction blocks being connected to one or more cooling devices with one or more temperature control devices being associated with the one or more cooling devices.

1 20. The apparatus of claim 18, wherein the user interface has a first display
2 screen having a first display window where a temperature vs. time graph for the study is displayed
3 and a plurality of a user input display windows which display user inputted information including
4 the predetermined temperature profile and the predetermined study time period and the number of
5 reaction vessels.

1 21. The apparatus of claim 20, wherein the user interface includes a
2 (model fit window) where a selected model fit program is displayed and the kinetics data is fitted to
3 the desired kinetics model fit program to generate the temperature vs. time graph.

1 22. The apparatus of claim 18, wherein the controller includes a master
2 control display screen having simulated hot and cold reaction block displays which indicate locations
3 of the reaction vessels within each of the hot and cold reaction blocks.

1 23. The apparatus of claim 22, wherein the master control display screen
2 has a thermometer display associated with each of the hot and cold reaction blocks, each
3 thermometer display having a graphic thermometer display indicating a temperature of the associated
4 one of the hot and cold reaction blocks and a second display window for numerically indicating the
5 temperature of the associated one of the hot and cold reaction blocks.

1 24. The apparatus of claim 20, wherein the robotic device includes a
2 gripping mechanism for gripping and transferring one reaction vessel from the hot reaction block
3 to the cold reaction block at one of the predefined transfer times.

1 25. The apparatus of claim 24, wherein the gripping mechanism includes a
2 first finger and a second opposing finger with a space therebetween, one reaction vessel being
3 disposed within the space and held between the first and second fingers during the transfer of the one
4 reaction vessel from the hot reaction block to the cold reaction block.

26. The apparatus of claim 24, wherein the controller includes a master
clock and a count-down clock, the master clock displaying a remaining time left in the study and the
count-down clock displaying a remaining time before the next transfer of one of the reaction vessels.

1 27. The apparatus of claim 1, wherein reaction data for each reaction vessel
2 is used to generate a single data point.
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28. A method of performing reaction kinetics studies and collecting data

using an automated apparatus, the method comprising:

providing the automated apparatus, the apparatus including:

a plurality of reaction blocks including at least one hot reaction block for heating one or more reaction vessels and at least one cold reaction block for cooling the one or more reaction vessels after heating thereof;

a robotic device for transferring one reaction vessel from one hot reaction block to one cold reaction block; and

a controller having a user interface and being in communication with the robotic device;

entering a first input using the user interface, the first input corresponding to a number of reaction vessels used in the study;

entering a second input using the user interface, the second input corresponding to a predetermined temperature profile which represents the temperature of at least one of the hot reaction blocks over a time period of the study;

entering a third input using the user interface, the third input corresponding to the time period of the study beginning with a start time and ending with a stop time;

transferring the reaction vessels at predefined transfer times, the predefined transfer times being calculated using the first and third inputs, each reaction vessel being transferred

20 from one hot reaction block to one cold reaction block by the robotic device which receives
 21 command signals from the controller; and
 22 collecting kinetics data including at least a temperature of the hot reaction
 23 block at each transfer time and a sampling time indicating when each reaction vessel transfer
 24 occurred.

1 29. The method of claim 28, wherein transferring the reaction vessels
 2 comprises:

3 sending a signal from the controller to the robotic device causing a gripping
 4 mechanism of the robotic device to be positioned at a predefined coordinate location relative to one
 5 of the hot reaction blocks where the gripping mechanism is instructed to securely grasp one of the
 6 reaction vessels, the one reaction vessel then being delivered to one of the cold reaction blocks for
 7 storage thereat.

1 30. The method of claim 28, wherein the gripping mechanism includes a
2 first finger and a second finger with a space therebetween, one reaction vessel being disposed within
3 the space and held between the first and second fingers during the transfer, the gripping mechanism
4 being operated by:

5 toggling a predetermined pressure between first and second lines, the gripping
6 mechanism closing about the one reaction vessel when the pressure is applied to the first line and
7 the second line is vented, the gripping mechanism being opened to release the one reaction vessel
8 by applying the pressure to the second line with the first line being vented.

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31. The method of claim 28, wherein the at least one hot reaction block is
heated by a heating device, the heating device having a temperature control device and a temperature
monitoring device associated therewith, the temperature control device maintaining the temperature
of the at least one hot reaction block according to the first input.

1 32. The method of claim 28, further including:
2 entering a fourth input using the user interface, the fourth input representing
3 a model fit program to which the kinetics data is fitted to generate a representative temperature vs.
4 time graph.

1 33. The method of claim 32, wherein the model fit program is one of an
2 isothermal temperature model or a non-isothermal temperature model.

1 34. The method of claim 31, further including:
2 entering a fifth input using the user interface, the fifth input being a value for
3 the number of reaction vessels to be transferred at each predefined transfer time; and
4 transferring the reaction vessels according to the fifth input.

35. The method of claim 32, wherein the fourth input is selected from the
group consisting of a logarithmic fit, a reciprocal fit, a linear fit, an exponential fit, and a power
function of time fit.

36. The method of claim 28, further including:
2 performing multiple kinetics studies in parallel by having at least one hot
3 reaction block and at least one cold reaction block associated with a first run and at least one hot
4 reaction block and at least one cold reaction block associated with a second run, wherein at least one
5 of the first, second, and third inputs is different between the first and second runs.

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1 37. The method of claim 28, further including:
2 performing multiple kinetics studies in parallel by having at least one hot
3 reaction block and at least one cold reaction block associated with a first run and at least one hot
4 reaction block and at least one cold reaction block associated with a second run, wherein at least one
5 of the first, second and third inputs is different between the first and second runs, wherein the first
6 run is an isothermal run and a the second run is a non-isothermal run.

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